

Electron Impact Ionisation and Fragmentation of Biofuels

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Experimental and theoretical studies on electron impact ionisation and fragmentation of the biofuels methanol, ethanol, 1-propanol and 1-butanol, have been performed in this work. The experimental measurements of the cations created in electron impact ionization and fragmentation of these alcohols were observed using a Hiden Analytical quadrupole mass spectrometer (EPIC 300), with a mass resolution of 1 amu. The mass spectrum recorded at an incident electron energy of 70 eV, reveals the probability of forming different cations by either direct ionization or dissociative ionization. Individual partial ionization cross sections (PICS) for the main cationic fragments observed of each alcohol were also registered at electron energies in the range of 10-100 eV. Total Ionization Cross Sections (TICS) were obtained from the sum of the measured PICS, for nearly all cations measured, and are compared to relevant data reported in the literature. In addition, theoretical TICS were calculated using the Binary-encounter Bethe (BEB) and independent atom model with the screening corrected additivity rule (IAM -SCAR) methods. Good agreement between current measured and calculated TICSs and corresponding earlier results was typically found, as it is shown in figure 1. Also, appearance energies (AEs) and Wannier exponents for the most intense cations formed in electron collisions with the studied alcohols were obtained. Where possible, those results are compared to those from an earlier investigation [1].

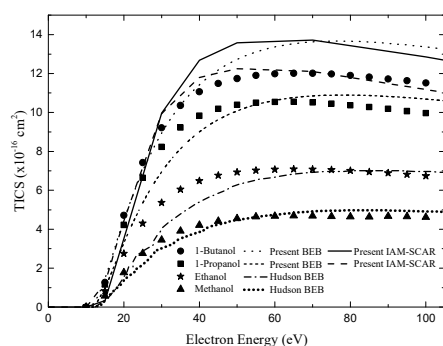


Fig 1: The comparison of the absolute total ionization cross of methanol, ethanol, 1- propanol, 1-butanol in 10-100 eV impact electron energy range.

Work at Brazil supported by FAPEMIG, CNPq and FINEP, in Australia by the Australian Research Council and at Spain by the Ministerio de Economía, Industria y Competitividad.

References

- [1] James E. Hudson *et al.* *Phys. Chem. Chem. Phys.*, **5**, (2003), 3162–3168.